AFOSR-TR-97-0720

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
		FINAL 01 Apr 96 to 31 Mar 97

4. TITLE AND SUBTITLE
COMPUTER SIMULATIONS OF LOW TEMPERATURE HIGH ENERGY DENSITY MATERIALS

5. FUNDING NUMBERS
F49620-96-1-0129
2303/FS
61102F

6. AUTHOR(S)
Dr Gregory A. Voth

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Dept of Chemistry
University of Pennsylvania
Philadelphia PA 19104-6323

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AFOSR/NL
110 Duncan Avenue Room B115
Bolling AFB DC 20332-8050

Dr Michael R. Berman

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION AVAILABILITY STATEMENT
Approved for public release;
distribution unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*
Solid hydrogen doped with energetic impurities may form the basis for HEDM to be used in rocket propulsion. A key research priority was therefore the largescale computer simulation of impurity diffusion and recombination in HEDM in order to better understand the reasons for its stability, or instability, as the case may be. The recombination of these atomic impurities is an extremely exothermic reaction, and therefore thermodynamically favored. Theoretical developments within our research group allowed for the (otherwise impossible) quantum dynamical simulation of these systems which was necessary to properly treat the problem. Classical molecular dynamics simulations, while less computationally challenging, predict qualitatively incorrect properties for low temperature liquid and solid hydrogen because of the highly quantum nature of hydrogen matrix, and are therefore inadequate.

19971217 015

14. SUBJECT TERMS

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
(U)	(U)	(U)	(UL)

To: Michael Berman@ngNL
From: Gregory A. Voth <voth@chemistry.chem.utah.edu>
Cc:
Bcc:
Subject: Final Technical Report: First Part
Attachment:
Date: 10/22/97 12:00 AM

AFOSR Final Report

Computer Simulations of Low Temperature High Energy Density Materials (F49620-96-1-0129)

Gregory A. Voth
Department of Chemistry
University of Pennsylvania
Philadelphia, PA 19104-6323

Introduction: Low Temperature HEDM Simulations

Solid hydrogen doped with energetic impurities may form the basis for HEDM to be used in rocket propulsion. A key research priority was therefore the largescale computer simulation of impurity diffusion and recombination in HEDM in order to better understand the reasons for its stability, or instability, as the case may be. The recombination of these atomic impurities is an extremely exothermic reaction, and therefore thermodynamically favored. Theoretical developments within our research group allowed for the (otherwise impossible) quantum dynamical simulation of these systems which was necessary to properly treat the problem. Classical molecular dynamics simulations, while less computationally challenging, predict qualitatively incorrect properties for low temperature liquid and solid hydrogen because of the highly quantum nature of hydrogen matrix, and are therefore inadequate.

The immediate goal of the research project was to calculate directly from largescale computer simulation the relevant rates for the impurity recombination process. In low temperature hydrogen HEDM, quantum effects are enormous, so a highly specialized method is required for these demanding computer simulations.

This grant lasted only for one year at the University of Pennsylvania because the P.I. moved to the University of Utah.

Summary of Key Results:

The primary result was the largescale quantum calculation of the intrinsic lithium impurity recombination rate in para-hydrogen at 4K.

Gregory A. Voth, Ph.D.
Professor of Chemistry and Director of the Henry Eyring Center for Theoretical Chemistry

Department of Chemistry
University of Utah
315 S. 1400 E. RM Dock